A Novel Chinese Traditional Medicine Prescription Recommendation System based on Knowledge Graph

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A Novel Chinese Traditional Medicine Prescription Recommendation System based on Knowledge Graph

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Abstract. As the traditional Chinese medical approach, Chinese medicine plays an extremely important role in the field of medical treatment. With the development of computers, people tend to acquire medical knowledge from the Internet in daily life. Because of the complexity of online Chinese medicine knowledge, nowadays there is no good way to organize the existing knowledge to provide convenience for doctors and patients. This paper introduces the study on the recommendation system based on the Knowledge Graph (KG). Firstly, it conducts extraction of entities such as Traditional Chinese Medicine (TCM) diseases, prescription, Chinese herbal medicine, symptoms, etc. Secondly, it transforms KG into vector space using Node2vec. At last, based on the similarities between vectors the provided system recommends prescription by adopting the diagnostic process of Traditional Chinese Medicine. The result shows that the Hit Ratio (HR) of the recommend system is as high as 80%.

1. Introduction

Traditional Chinese Medicine (TCM), the treasure of the Chinese nation civilization, has thousands of years of history and has been used for medical and health services widely in China and pan-Chinese culture regions. TCM is accepted for its effective and abundant medical function and reasonable price. Compared with Western medicine, TCM has the following main advantages: (1) TCM has few side effects, since it can be used externally. (2) TCM has less damage to gastrointestinal tract. (3) TCM has light stimulation on kidney and liver. Besides, TCM cannot only be used to treat illness but also preserve health for almost everybody.

With rapid development of big data nowadays, artificial intelligence will play an unlimited role in the Internet & medical field. Recommendation system is becoming more and more important in solving problems of information explosion.

Researchers hope that people can use Data Mining technology to collect more data in the field of health care and make full use of them to benefit millions of patients. Therefore, the author tries to establish a precise recommendation system of Chinese medicine prescriptions based on the knowledge graph，the precise recommendation algorithm and the traditional Chinese medicine theory.

Nowadays, there are still many problems in the medical recommendation system:

1) It is called Information overload that the information is too large to be used effectively by individuals or systems and causes malfunctions [1].

2) Personalized medical recommendation based on user collaborative filtering algorithm is adopted. Due to the variability, complexity and diversity of personal medical behavior, the accuracy of system recommendation is not enough to be put into service.
3) Because of the complexity and diversity of traditional Chinese medicine (TCM), the existing medical recommendation system is mainly in the field of Western medicine, recommending doctors, and there is almost no recommendation system for TCM prescriptions.

TCM medical records provide first-hand information for TCM therapeutics, which is very helpful for the promotion and development of basic theories of TCM and progress and supplement of TCM and formulaology. In order to be more accurate to realize the precision recommendation of TCM prescriptions, this paper crawls and processes the TCM case data from the authority website "National Service Platform for Academic Experience of Famous and Old TCM", and constructs a thesaurus based on the TCM knowledge, extracts the entities and relationships in medical cases, and constructs a knowledge map of TCM case.

Knowledge Graph is an emerging technology for massive knowledge management and intelligent services in the big data era. It can capture and present the intricate relationships among the domain concepts, and connect the fragmented pieces of knowledge in various information systems. Considering excellent expansibility, interpretability and analytical ability of graph structure, this paper organizes the entity of prescription, the entity of syndrome of prescription treatment, the attribute of syndrome, and the relationship among the entities as a graph. Figure 2 shows in detail the entities such as prescriptions and their relationships in the recommendation system.

Prescriptions and disease syndromes are stored in the form of nodes, which contain the content information of corresponding entities, such as tongue coating, tongue texture, pulse and so on. The relationship is the edge of the nodes. In this paper we present our content-based recommendation system which is capable to incorporate several information source types. The knowledge base is introduced as a directed, labeled, restricted hypergraph. We also define a recommendation calculation method which provides higher quality recommendations than collaborative filtering does. This way we prove on a working example that the involvement of an increased and heterogeneous amount of information sources can lead to higher quality recommendations.

This paper aims to design and implement a precise recommendation system for traditional Chinese medicine based on machine learning algorithms and Classics of traditional Chinese Medicine. The main contributions are: 1) propose a Knowledge Map-based recommendation algorithm for Chinese medicine prescriptions, which uses reptiles and knowledge maps to store unstructured natural languages including ancient Chinese medicine books and clinical medical records structurally and semantically. 2) precisely recommend corresponding prescriptions according to the extracted patients' symptoms. 3) Based on the ideas put forward, this paper implements the prototype system of the recommendation system of TCM medical records, and verifies the feasibility of the method with real clinical data of TCM. The accuracy rate of recommendation is more than 85%.

This paper is organized as the follows. Section 2 contains serval recommendation related techniques, which operate with graph related representation methods. In Section 3 we provide an overview of the provided recommendation system including a formal definition of our knowledge base. Section 4 describes our calculation method, which is based on spreading activation. In Section 5 we describe how we evaluated our pivot method and present our evaluation results. Section 6 concludes the paper and gives an insight into our plans for the future.

2. Related word

2.1. Recommendation System

Recommendation system helps people cope with information overload by recommending related items according to personal preferences. According to the different data used in traditional recommendation systems, recommendation algorithms can be divided into collaborative filtering recommendation [2], content-based recommendation [3], hybrid recommendation [4], etc. Recently, most recommendation

technologies have been widely used in online art recommendation [5], movie, video recommendation [6], and helping scientists find relevant academic materials [7].

With the development of recommendation system, people are not only satisfied with the analysis of users' historical behavior for modeling, but also devote themselves to solving problems of cold start and extremely sparse data by various methods. For example, the similarity model of hybrid projects designed by combining the two methods: computing similarity based on co-evaluation items or using all rating information to calculate similarity. Junpeng Guo has realized the balance between forecasting progress and forecasting efficiency in this paper [8]. Besides, the research work [9] provides the improved collaborative filtering algorithm using normalized user rating vectors and item rating vectors as inputs of the neural network, and a batch normalization technology is used in each layer. The experimental results show that the algorithm can be well operated online without additional complexity and performance sacrifice. Besides, the research work [10] proposed an improved CBF algorithm (content-based filtering) using multi-attribute networks to effectively reflect multiple attributes when calculating correlation, in order to recommend items to users

2.2 Knowledge Graph

Knowledge Graph technology can extract entity, entity attributes' information and the relationship between entities from Internet web pages, aiming at solving the problems of automatic question answering, personalized recommendation and intelligent information retrieval. With the rapid development of knowledge atlas in recent years, Question Answering System based on knowledge graphs has attracted wide attention of the industry [11]. This kind of question answering system adheres to the design idea of coding first and then comparing, that is, coding the content of the question and knowledge map into a unified vector space, and then calculating the similarity between the question and the candidate answer in the vector space. It has been proved that this method is simple but effective and operable.

Knowledge graphs have been applied to recommend music artists, movies, books, and tourist attractions by constructing rich knowledge maps of tourism space-time. Two main shortcomings have been successfully solved: the fusion of multiple heterogeneous data and the lack of spatiotemporal characteristics [12]. Knowledge graphs can also be used in medical field. At present, automatic medical knowledge graphs based on semantic analysis has been proposed, which can be used in personalized treatment recommendation [13]. In addition, T-Know, a knowledge service system based on knowledge graphs, realizes a knowledge retrieval system supporting human-computer interaction from clinical records and clinical medical guidelines.[14]

Compared with the previous work, the innovation of this paper is to make full use of the advantages of KG, take KG as a part of the recommendation system, store the data of traditional Chinese medicine structurally and semantically, and propose a precise content-based recommendation algorithm according to the characteristics of disease-based treatment of traditional Chinese medicine.

2.3 Traditional Chinese Medicine

Traditional Chinese medical data has characteristics of volume, variety, speed and accuracy, which brings challenges to the storage, transmission and processing of emerging medical data. Moreover, the developed data processing technology provides an opportunity to use medical data to help clinicians in many applications, such as medical DSS (decision support system) [15], edge detection in medical diagnose [16], drug discovery analysis [17] and so on. Knowledge graphs of traditional Chinese medicine (TCM) is a knowledge graphs system based on TCM language system. Filled with existing database resources, knowledge graphs can enhance the connectivity of TCM knowledge resources, support TCM users to browse domain knowledge resources at the conceptual level and discover potential links between TCM concepts or knowledge [18].

At present, the specific research of TCM knowledge graphs mainly focuses on the knowledge organization method in TCM field, the storage and query of large TCM knowledge graphs, the development of TCM Knowledge acquisition technology based on TCMLS (Traditional Chinese

Medicine Language System). In addition, researchers design and realize the retrieval and browsing methods of knowledge graphs that meet actual needs in the field of traditional Chinese medicine. The knowledge graphs will be embedded in search and Wiki systems to provide knowledge services [19]. The purpose of this paper is to make a recommendation system which can be used in medical field and life service on the basis of previous research on the basis of previous technologies in TCM field. The recommendation system follows the basic principle of traditional Chinese medicine judging diseases according to diseases and then recommending prescriptions.

3. TCM Recommendation System

3.1. system review

The provided system in this paper is divided into three parts: data acquisition and processing module, KG construction module and recommendation module. The system is as shown in the figure 1.

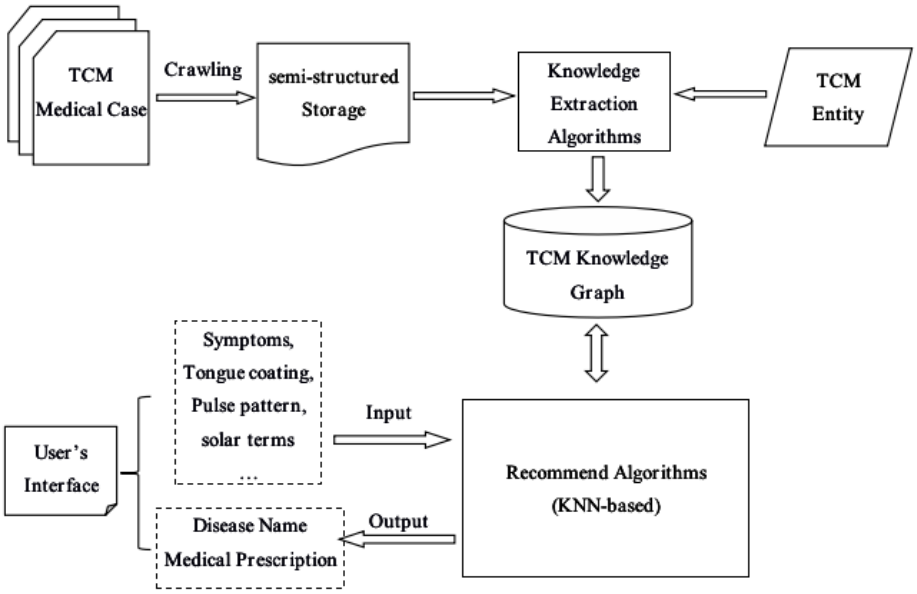

Figure 1. Figure with Overview of the TCM Recommendation System

Data acquisition module crawled clinical medical records from TCM web pages by using crawler technology. At the same time, data processing technology is used to preprocess the medical records data, including data cleaning (deleting incomplete data lack of important information of medical records, duplicate data, etc.), data standardization, and saving the processed data as text files. The KG construction module includes the extraction of TCM knowledge, the representation and storage of TCM knowledge. Knowledge extraction of TCM includes entity extraction and relationship extraction. The details of the Knowledge Graph is provided in sub-section 3.3. The recommendation module receives the user's input disease information and extracts the entity. At the same time, it obtains the semantic information of prescriptions and diseases based on knowledge atlas learning algorithm: node2vec. The symbolized entities and relationship are constructed into candidate set of vectors. The distance between the user's input disease entity and candidate prescriptions will be calculated, and the recommendation list of prescriptions is given in ascending sort order.

The following sub-sections will provide more details about each module.

3.2. TCM Data Acquisition

This section gives the method of data acquisition of this paper. The data acquisition of the recommendation system is divided into two parts: data of TCM medical record and entity data of TCM.

The entity data of TCM is collected from TCM classics and as the basic TCM terminology data it includes TCM prescription names, TCM disease names, TCM herbal medicine and so on. The function is to extract entity information from TCM medical records. The data of TCM medical record is the core data of this system, which includes TCM medical knowledge such as prescription names, doctor's names, department, patient information, TCM diagnosis, western medicine diagnosis, solar term, tongue coating, tongue texture, pulse signs, chief complaint, etc. The question to be answered by the recommendation system of TCM is to recommend suitable TCM prescriptions to patients according to the information of diseases such as diseases, tongue texture, tongue coating and pulse signs provided by patients or doctors, and to make preliminary judgments for patients' diseases. One of the core tasks of this paper is to extract the substantive knowledge of TCM medical records by using medical records data in order to build knowledge graph. The data of TCM medical record comes from the website of famous and veteran TCM, and the entity data of TCM comes from the thesaurus of Wanfang Medical Database.

This article uses crawlers to get data. The working process of the crawler is described as follows:

1) Send a request to the target site containing medical record data by using HTTP module, which includes: the request head, the request body, etc., and the request body contains the medical record index information to be obtained.
2) Get the response. The medical record data exists in the HTML format data.
3) Write HTML parsing template and extract medical record data.
4) Save data as text form.

3.3 TCM Knowledge Graph Construction

The construction of TCM knowledge graph is divided into two steps: extraction module of TCM knowledge, representation and storage module of TCM knowledge. The Extraction of TCM knowledge including entity extraction and relationship extraction. Firstly, the entity of this work is defined as disease of traditional Chinese medicine, prescription of traditional Chinese medicine, herbal medicine of traditional Chinese medicine and syndrome of traditional Chinese medicine. The relationship between entities is: the treat relationship between diseases and prescriptions, the consisting relationship between prescriptions and herbs, and the characterization relationship between diseases and symptoms. In this paper, the relationship between entities is relatively clear, so the focus is on how to extract the entities in medical records. The KG is as shown in the figure 2.

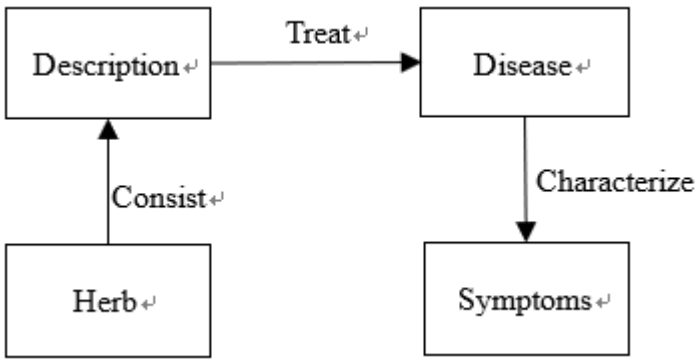

Figure 2. Figure with the scheme of the TCM Knowledge Graph

A. Knowledge Extraction Module

B. The knowledge extraction module is used to extract the four kinds of entities defined in Figure 2. In this paper, two methods are employed for entity extraction: 1) Entity extraction based on dictionary. 2) Entity extraction based on deep learning.

3.3.1. Entity extraction based on dictionary. There are two methods of entity extraction based on dictionary: String multi-mode matching and Word segmentation matching.

This paper combines maximal-matching and word segmentation matching in string multi-mode matching algorithm. Firstly, using maximal-matching, and then putting the extracted entity back into the result of word segmentation to see if it is "complete" (Words from maximal-matching at the beginning of a word do not form a word with the previous word in the result of word segmentation, and words at the end do not form a word with the latter word in the result of word segmentation either.) For example, "liver and kidney insufficiency", firstly look up the words beginning with "liver and kidney" which have length 4 and 2, then take four lengths of "liver and kidney insufficiency". If not in the dictionary, then take two lengths of "liver and kidney". If there is one in the dictionary, it hits.

However, the method based on dictionary has some shortcomings. It sometimes does not work to add words to a custom lexicon. If there are two words that contain a relationship and add a self-defined lexicon at the same time, the result of word segmentation is short words rather than long words. And in this experiment, some dictionaries lack some Chinese medicine terms which cannot be recognized, so this paper uses deep learning method to make up for the deficiency of dictionary-based method.

3.3.2. Entity extraction based on deep learning. In this paper, the serial entity extraction method mentioned in the literature [20] is used to realize the extraction of medical record entity. According to the characteristics of TCM texts, BiLSTM and CRF are designed to implement the "word" level and use BIO for annotation.

The first layer of the model takes the sequence of Chinese characters as the initial input. The second layer is the embedding layer, which maps each word in the input word sequence of the first layer into corresponding vectors. Word2vec is used for pre-training to get the word vector, which is used as the initial parameter of embedding layer. The third layer is a two-way long-term and short-term memory (LSTM) network structure. The dimension of LSTM is set to half of the output dimension of embedding layer. The bidirectional circular application network is used to take full account of the context information and get the context representation vector of the current word. Finally, CRF is used to obtain the annotation sequence according to the sequence of context representation vectors. According to the context representation vectors of each word, the probability of each word labeling target can be obtained directly from the softmax of classification algorithm. In order to prevent over-fitting, dropout regularization mechanism is introduced into the training stage model and placed at the output of BiLSTM layer.

3.3.3. Knowledge Representation and Storage Module. When entities are extracted, they should be represented and stored. Three-tuple data were extracted from clinical medical records of traditional Chinese medicine. The data format of the triple is defined here as R (e1, e2), which indicates that entity e1 is related to entity e2. The knowledge representation module standardizes the representation of knowledge tuples. This knowledge map of TCM is mainly aimed at the knowledge of TCM diseases and prescriptions.

Neo4j graph database is used as database engine for knowledge storage. Referring to the definition of knowledge representation stage before storage, two types of node labels, disease and prescription, and directed treat relationship labels, are defined in graph database. In order to ensure that no more than one node has the same specific label or unique constraint attributes, for each node a unique constraint is created. The entity and relationship information of TCM is
imported into Neo4j graphics database through CQL statement, and the duplicate relationship is removed.

3.4. KG-based recommendation algorithm:

In this section, we first get the vector representation from the TCM knowledge graph. Then, we employ a KNN-based algorithm to recommend the TCM prescriptions.

3.4.1. Knowledge Map Learning Based on Node2vec. In this paper, we use Node2vec algorithm[21], which has good performance in projecting nodes and edges into low-dimensional vector space based on KG and enhancing the semantic information of disease and prescription scoring matrix in recommendation algorithm. According to the definition of Node2vec algorithm, for a triple R (e1, e2) in the knowledge map s, a random walk with parameters is defined on the graph, and the sequence of nodes is obtained by BFS and DFS. Then the vector representation of nodes is obtained by Word2vec method for the sequence.

Node2vec is realized in three steps. The first step is to calculate the transition probability matrix, the second step is to sample and generate training sample sequence, and the third step is to optimize with gradient descent.

3.4.2. KG-based Recommendation algorithm. K-Nearest Neighbor (KNN), is one of the commonly used methods in data mining technology. The so-called K nearest neighbor means that each sample can be represented by its nearest K neighbors. The core idea of KNN algorithm is that if most of the K most adjacent samples in feature space belong to a certain category, the sample also belongs to this category and has the characteristics of samples in this category.

The patient takes the Chinese expression of the disease and symptoms as the input of the system. For example, on the fifth day after the vernal equinox, the left facial leukoplakia lasts for more than one month, the tongue is red, the tongue coating is less, the pulse pattern is stringent, and abdominal pain is prone. In the output list of the algorithm, there are recommended prescriptions arranged in descending order of symptoms similarity. The system is designed to return to the recommended list containing ten recommended prescriptions for system users to refer to. Each entry contains the prescription name and solar terms, tongue coating, tongue texture, pulse, engraving syndrome, traditional Chinese medicine diagnosis, western medicine diagnosis, traditional Chinese medicine symptoms, doctor's advice. The KG-based algorithm process is described as the following.

1) The system calls the existing data processing module to normalize Chinese input and extract keywords as valid information according to the constructed disease glossary.
2) Construct the patient's disease vector through node2vec, the feature dimension is 128.
3) Computing the similarity between the input vector and all items in the candidate set of prescription-disease vectors constructed by node2vec algorithm by calculating the Euclidean distance between them.
4) Sorting all distances in ascending order
5) Choosing the top10 vectors with the smallest distances, we can get the prescriptions which are most consistent with the patient's disease.

4. Experiments and Results

4.1. Implementation

This paper implemented a protype of the KG-based system as presented in previous sections. We provided some details of the implementation here.

4.1.1. Entity extraction algorithm based on BiLSTM-CRF. The probability of dropout layer is set to 0.5. The model uses back propagation algorithm to fit the training data, and updates the parameters for each training sample. Adam gradient descent algorithm is adopted in this paper. The learning rate is 0.001 and batch_size is 16. Fifty rounds of training are conducted. LSTM basic unit select no peephole. The initial bias of forgetting gate is 1. Independent forgetting and input thresholds are adopted. The CRF model defines the window size of the context feature is 3. BiLSTM-CRF model obtains the context information of words through BiLSTM layer, which can receive the context features more completely and has the ability of fitting non-linearity.

4.1.2. Node2vec. Node2vec takes DFS neighborhood and BFS neighborhood into account, and still uses random walk to obtain the nearest neighbor sequence of vertexes, but node2vec uses a biased random walk. Node2vec introduces two hyper-parameters P and Q to control random walk. Parametric P controls the probability of repeated visits to newly visited vertexes, and Q controls whether random walk is outward or inward. In this paper, the vector dimension is 128, walk-length is 80, num-walks is 10, window-size is 10, P is 1, and Q is 1. The graph defaults to undirected and weightless.

4.1.3. KNN. In this paper, KNN uses Euclidean distance to measure the similarity between two vectors (symptoms and prescriptions). Using the cross-validation method in sklearn, 20 percent of data set about 90 data were randomly sampled from the symptoms set and calculated by KNN. The calculated European distance was arranged in ascending order, and the first K prescriptions were selected as the recommended prescriptions.

4.2. Data Set and Measurement criteria

The data comes from clinical medical records of traditional Chinese medicine. In the experiment of entity extraction algorithm, in order to reduce the computational complexity of model training and speed up training, long sentences are divided into short sentences with no more than 50 words. The experimental corpus was constructed by dictionary matching and manual proofreading, and the dictionary of TCM prescriptions in Wanfang TCM knowledge base was selected. There are four kinds of naming, traditional Chinese medicine, prescriptions symptoms and diseases entities. Data sets are labeled by BIO. In terms of corpus, the latest Chinese Article corpus provided by Wikipedia and the corpus of Chinese classics are used as the training corpus of Word2vec. In the constructed TCM Knowledge graph, there are 1709 prescriptions in the training set, 451 diseases. Our recommendation algorithm is measurement on these prescription and disease. In the experiment, we adopt Hit Ratio (HR) to evaluate the performance of this algorithm. It is defined as the formulation.

$$HR@k = -\frac{NumberofHits@K}{|GT|} \tag{1}$$

In the above formulation, the denominator is the total number of test sets in each user's first K and the molecule is the sum of the number of test sets in each user's Top-k recommendation list. This index measures the recall rate. The larger the index, the better result.

4.3 Experimental Results

In this experiment, 451 patients' symptoms extracted from TCM clinical medical records were transformed into vector form. 20% of the disease vectors were randomly selected by Sklearn module to form a test set. Additionally, two indicators were defined to evaluate the results of the test set. The two evaluation indicators are:

Accuracy_hit: HR that can recommend the correct prescription

Recall_hit: HR that can push all correct prescriptions for diseases

With the increase of K, both the recall_hit and accuracy_hit increase gradually. The experimental results are shown in the figure 3.

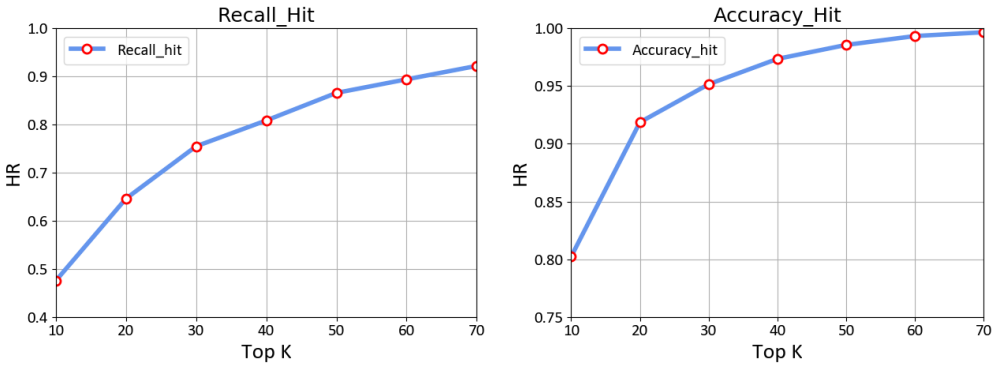

Figure 3. Figure with Hit Ratio of the TCM recommendation algorithm

4.4. Discussion

The algorithm and recommended system in this paper are suitable for TCM prescription adjuvant. By using a large amount of unstructured medical knowledge, TCM medical atlas can be automatically constructed. The knowledge atlas can be translated into the corresponding vectors of the entities, and related prescriptions can be recommended based on the knowledge atlas according to the patient's symptoms. The system can assist medical personnel in dispensing medicines for patients' condition. The medical manpower is saved to the greatest extent. Meanwhile, the system emphasis more on interaction. The limitation of the provided algorithm is it could be be unpredictable problems in practical application because of the complex and changeable situation of medical treatment and traditional Chinese medicine

5. Conclusion

There are a lot of unstructured TCM data on the Internet. Based on the knowledge of TCM diagnosis and treatment, this paper designs a system which can be used by doctors and patients to help recommend related prescriptions according to the disease and symptoms by linking three modules: automatic construction of knowledge graph module, transformation from knowledge graph to vector space module and recommendation according to symptoms' vector. The experimental results show that the proposed algorithm is highly accurate. The target entity extracted in this paper is limited to four kinds of entity: Chinese medicinal herbs, prescriptions symptoms and diseases. Expanding the types of entities and improving the recommendation efficiency are the next key work.

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